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Title: CartaBlanca

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Intended for: For general distribution to advertise CartaBlanca capabilities.

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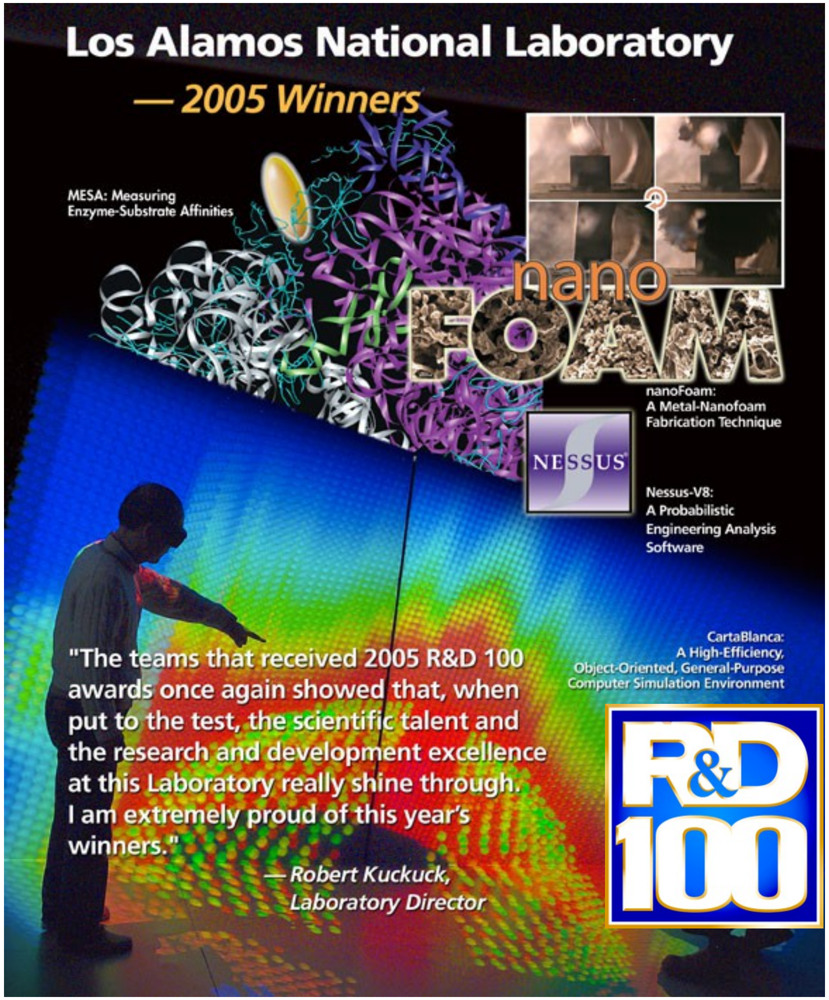
What is CartaBlanca

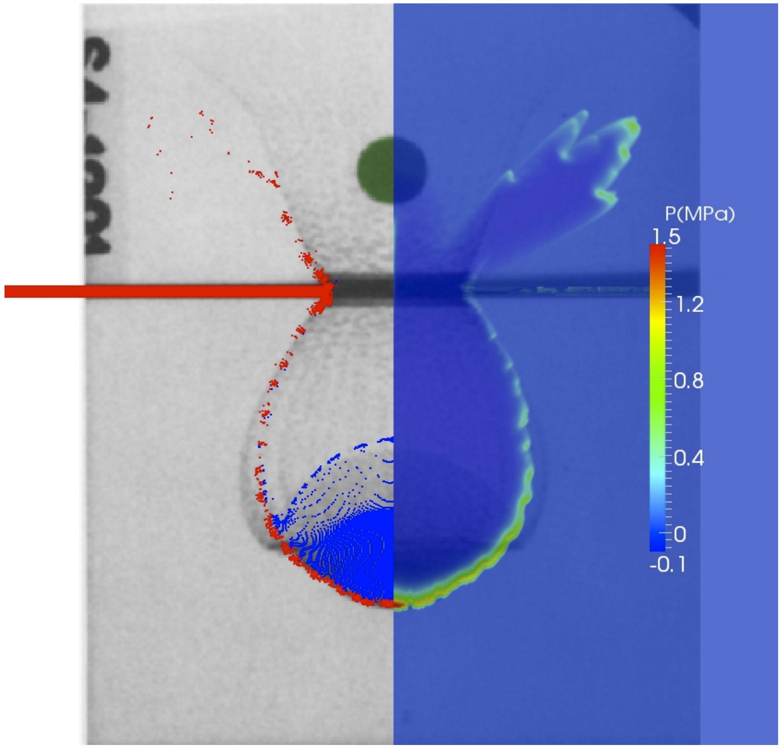
http://www.lanl.gov/projects/CartaBlanca/

CartaBlanca: **A High-Eff ciency, Object-Oriented, General-Purpose Computer Simulation Environment**

- A multi-physics numerical simulation package.
- Based on advanced multi-material interaction theory.
- Implemented with modern numerical methods.
- Works with any mesh and internals.

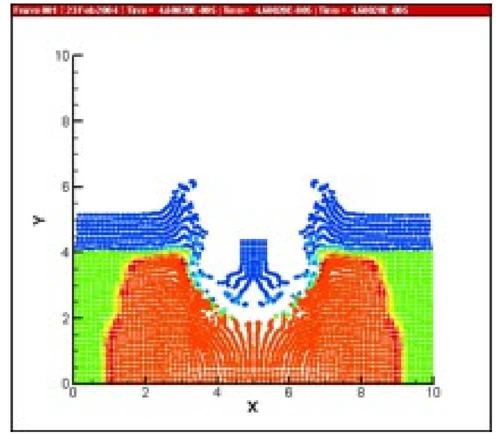


Solid to fluid transition with chemical reaction

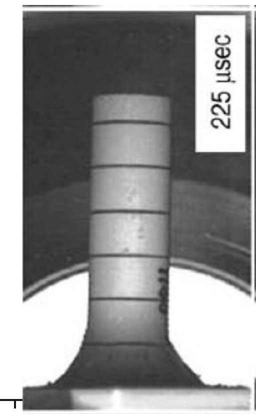


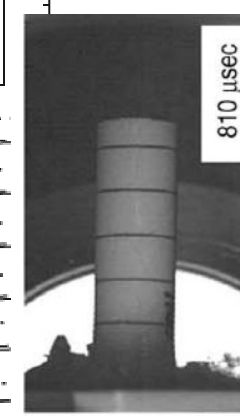
It starts with solid-solid interaction in air. It goes through transition from a solid phase to a disperse phase, and becomes a disperse multiphase flow.

Ma, X., Zhang, D.Z., Giguere, P. T. & Liu, C., 2013, , *International Journal of Impact Engineering.* 54, pp 96-104.



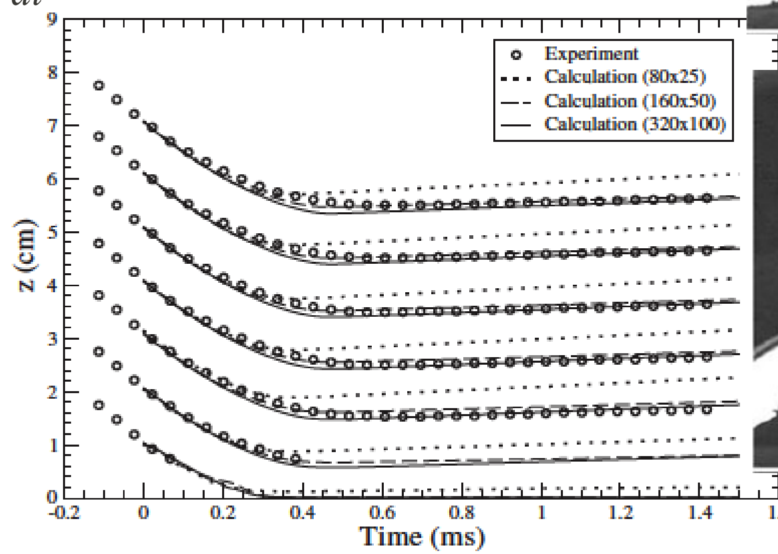
Chemical reaction (HE burn) triggered by an impact on a brittle material.





The impactor is viscoelastic:

$$\frac{d\boldsymbol{\sigma}}{dt} - \boldsymbol{\Omega}\cdot\boldsymbol{\sigma} + \boldsymbol{\sigma}\cdot\boldsymbol{\Omega} = -\frac{\boldsymbol{\sigma}}{\tau} + \lambda\, tr(\dot{\boldsymbol{\varepsilon}})\boldsymbol{I} + 2G\,\dot{\boldsymbol{\varepsilon}}\,.$$



Successful CartaBlanca Projects

Traditional fluid dynamics

- Fluidized bed for chemical industry.
- Heat and mass transfer with uranium and hydrogen reaction for nuclear reactors.
- Nuclear fuel separation in centrifugal contactors.
- Chemical reaction and evaporation in porous material for homeland security.
- Reacting multiphase flow in porous geo-material for oil industry.

Advanced multi-material interactions

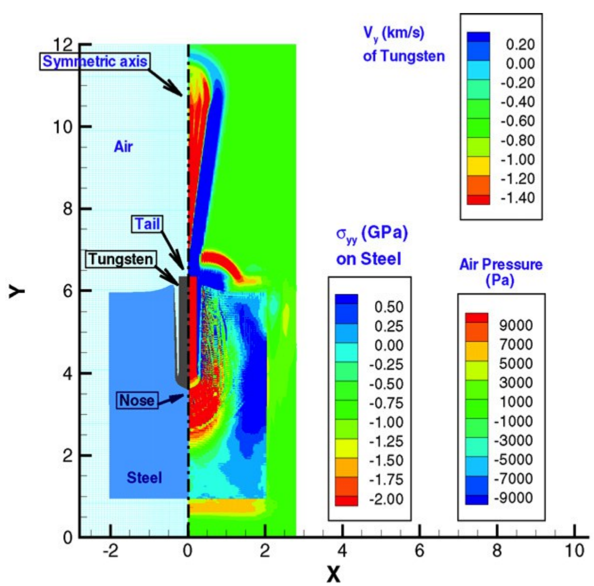
- Fluid-structure interactions in explosions.
- Hypervelocity impact in air or under water.
- Liquid fuel explosion for missile defense agency (MDA).
- Container strength effect on chemical explosions.
- Structure analyses under earth quake loading.
- Multiphase transonic flow and its corrosion effect on nozzles.

Model Equations

$$\frac{\partial \rho^{(i)} \boldsymbol{u}^{(i)}}{\partial t} + \nabla \cdot (\rho^{(i)} \boldsymbol{u}^{(i)} \boldsymbol{u}^{(i)}) = -\theta^{(i)} \nabla \cdot p + \nabla \cdot [\theta^{(i)} (\boldsymbol{\sigma}^{(i)} + p \boldsymbol{I})] - \boldsymbol{F}^{(i)},$$

where p is the fluid pressure, $\boldsymbol{F}^{(i)}$ is the interaction force among the materials. (Zhang and Prosperetti, JFM 1994, Zhang et al, IJMF 2007).

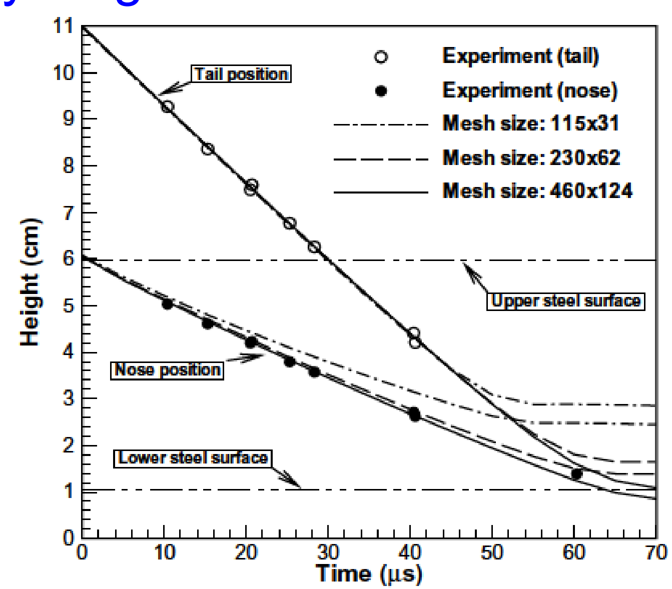
- In CartaBlanca the material stress is not limited to viscous or elastic stress. It can also be viscoelastic, plastic, ...
- We don't label a material by fluid or solid. Its constitutive relation determines whether it is solid, fluid or anything in between.



Continuous two-phase interaction

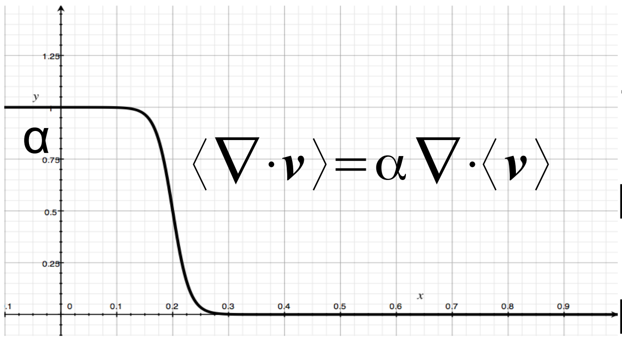
Large plastic deformation in solid.

Ideal gas model for air.



Ma X. Giguere, P.T., Jayaraman, B. & Zhang, D. Z., 2010, *Journal of computational physics*. 229, pp 7819-7833.
Zhang, D. Z., Zou, Q., VanderHeyden, W.B. & Ma, X. 2008, *Journal of computational physics*. 227, pp. 3159-3173

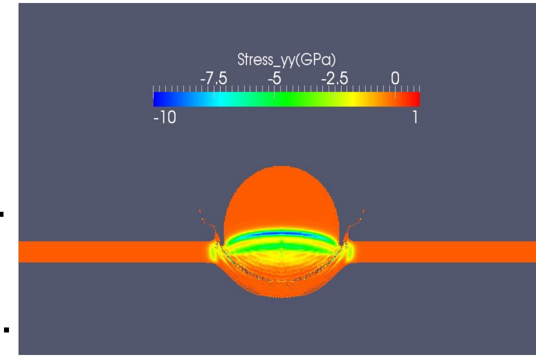
Solid to disperse flow transition

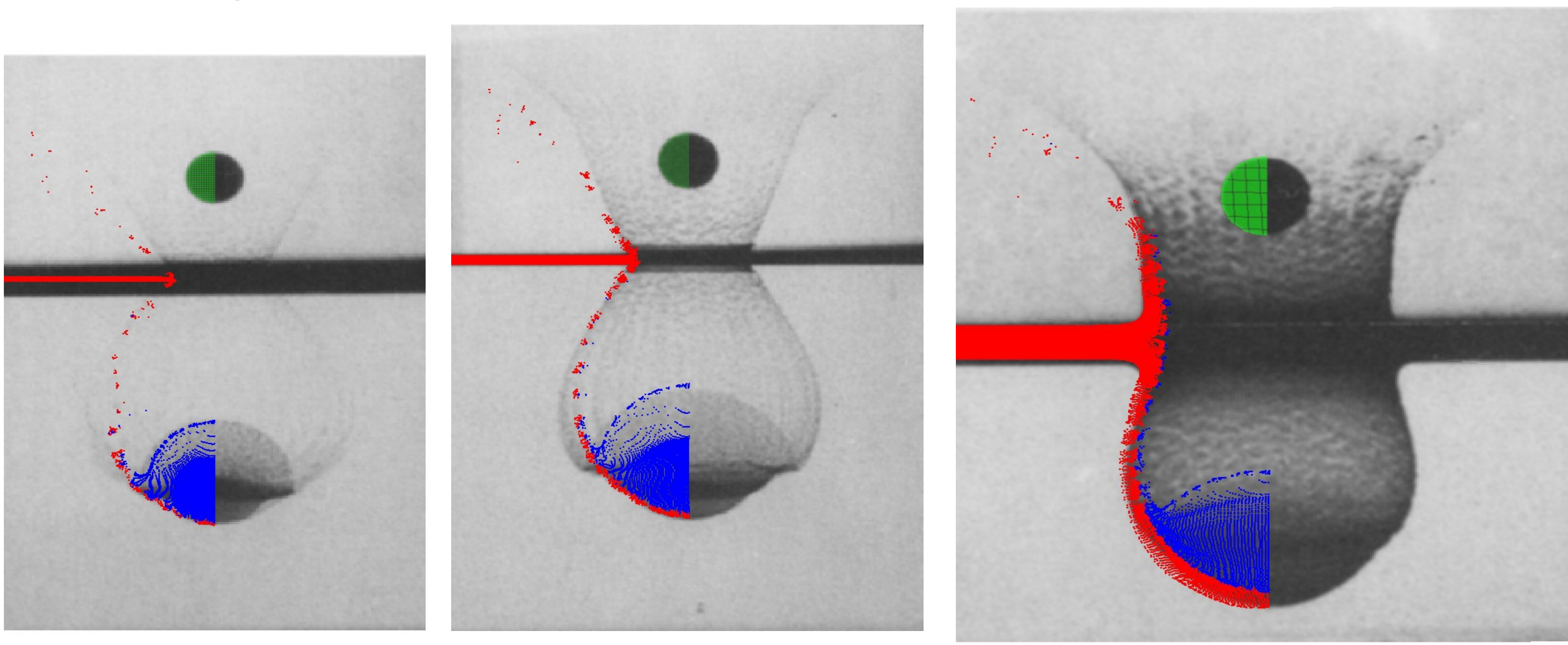


Relating velocity divergence to volumetric deformation.

For undamaged material $\alpha = 1$.

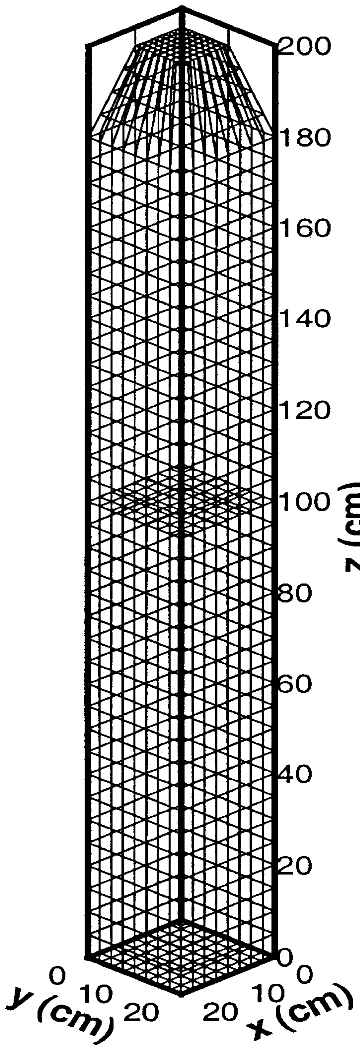
For completely damaged $\alpha = 0$.

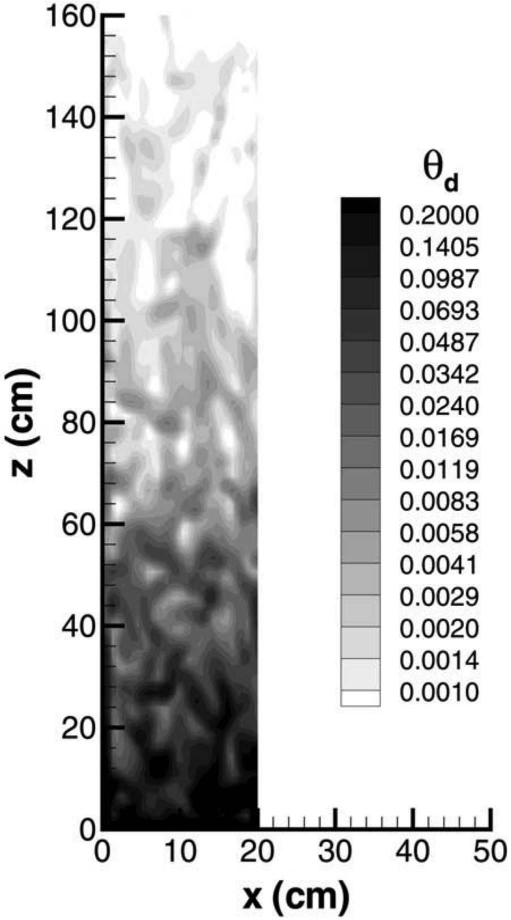


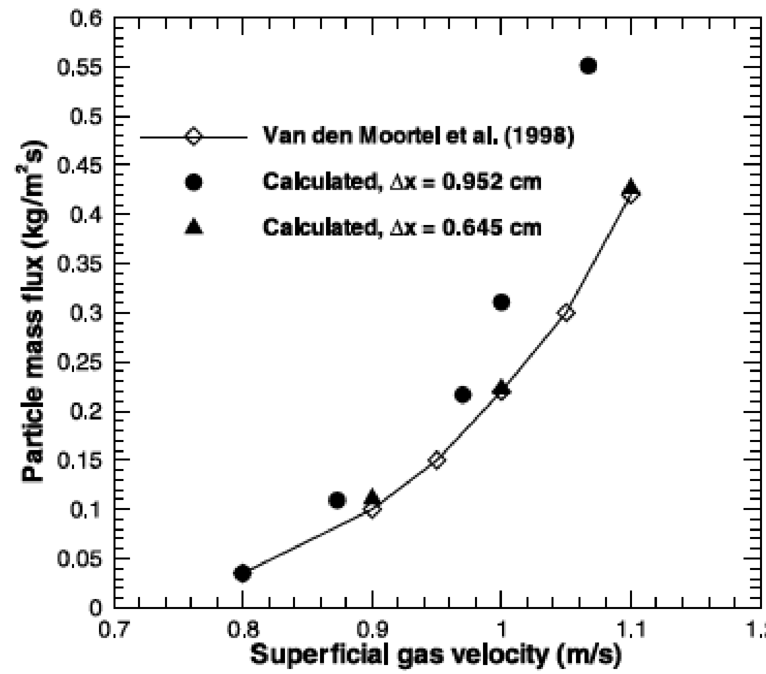


Blue: projectile material. Red: target material

Traditional two-phase flows – I
a fluidized bed

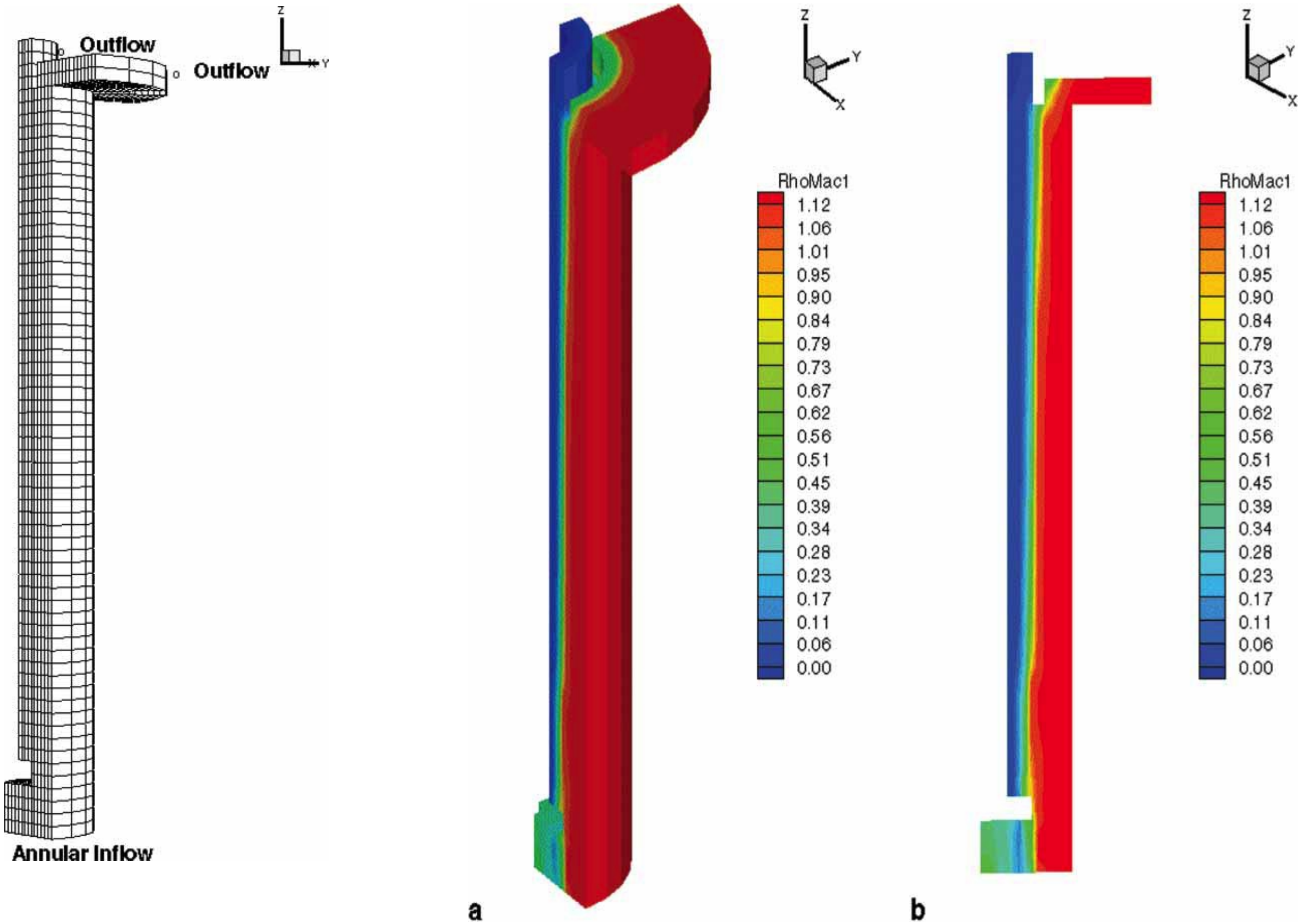






Zhang, D. Z. & VanderHeyden, W. B. 2001, *International Journal of Multiphase Flow*, 28, pp805-822.
Zhang, D. Z. & VanderHeyden, W. B. 2001, *Powder Technology* 116, pp133-141.

Traditional two-phase flows – II
(a centrifugal contactor, liquid-liquid two-phase flow)



Padial-Collins, N. T., Zhang, D.Z., Zou, Q. Ma, X. & VanderHeyden, W.B. 2006, *Separation Science and Technology*, **41**(6).

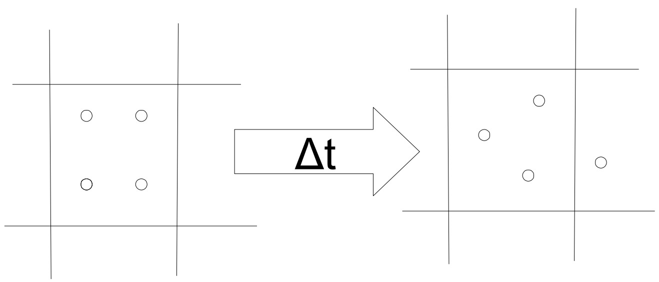
Material Point Method vs. Finite Element Method

$$m_i \frac{d\,\boldsymbol{v}_i}{dt} = -\int \boldsymbol{\sigma}\cdot\nabla S_i(\boldsymbol{x})\,dv + \int \rho\,\boldsymbol{g}\,S_i(\boldsymbol{x})\,dV + \int_{\partial v} S_i(\boldsymbol{x})\,\boldsymbol{\sigma}\cdot\boldsymbol{n}\,dS\,,$$

MPM

$$\int \boldsymbol{\sigma}\cdot\nabla S_i(\boldsymbol{x})\,dv = \sum_p v_p\,\boldsymbol{\sigma}_p\cdot\nabla S(\boldsymbol{x}_p)$$

where subscript p denotes material points that move across the Eulerian mesh.



Update particles: $\boldsymbol{v}_p^{n+1} = \boldsymbol{u}_p^{n} + \sum_i \Delta\,\boldsymbol{v}_i\,S_i(\boldsymbol{x}_p)$

Advection: $\boldsymbol{x}_p^{n+1} = \boldsymbol{x}_p^{n} + \Delta t \sum_i (\boldsymbol{v}_i + 0.5\,\Delta\,\boldsymbol{v}_i)\,S_i(\boldsymbol{x}_p)$

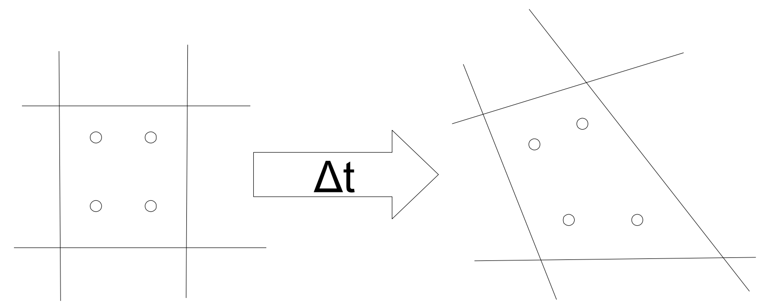
Update grid: $m_i\,\boldsymbol{v}_i^{n+1} = \sum_p m_p\,\boldsymbol{v}_p^{n+1}\,S_n(\boldsymbol{x}_p^{n+1})$

Mesh cells or elements are fixed.

FEM

$$\int \boldsymbol{\sigma}\cdot\nabla S_i(\boldsymbol{x})\,dv = \sum_g w_g J_g\,\boldsymbol{\sigma}_g\cdot\nabla S(\boldsymbol{x}_g),$$

where subscript g denotes Gauss integration points.



Gauss points are fixed on elements.

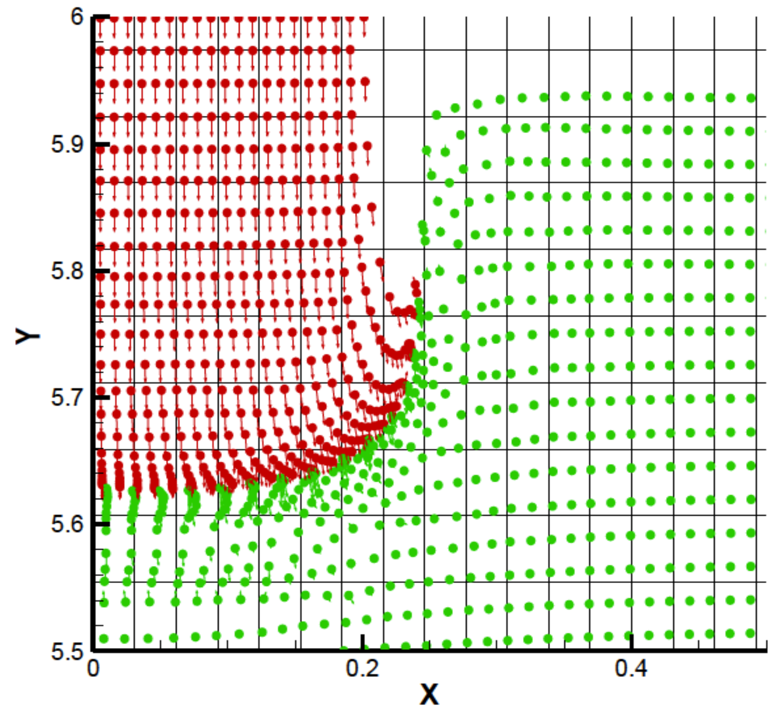
Elements are Lagrangian. They can be distorted for large material deformation.

Both the material points and the Gauss points are Lagrangian and can be used to track deformation history of the material. However, FEM has the difficulty of mesh distortion.

Material Point Method (MPM)

The material point method uses both Eulerian mesh and Lagrangian points. The Lagrangian points are also called material points, or particles.

- Particle-in-cell (PIC) method was first used by Frank Harlow in the 1960's. Nearest grid point interpolation is used.
- In the late 1980's, shape functions were introduced. The method is then called FLuid Implicit Particle method (FLIP).
- In the 1990's particle-in-cell method was re-formatted based on weak solutions to partial differential equations (or the virtual work theory). Since then the method is called the material point method (MPM).



- Effective for history dependent problems with **large** deformation.
- Can be used to track material interfaces. Very little numerical diffusion.
- It is more expensive than typical finite volume method and finite element method.

Compared to other codes

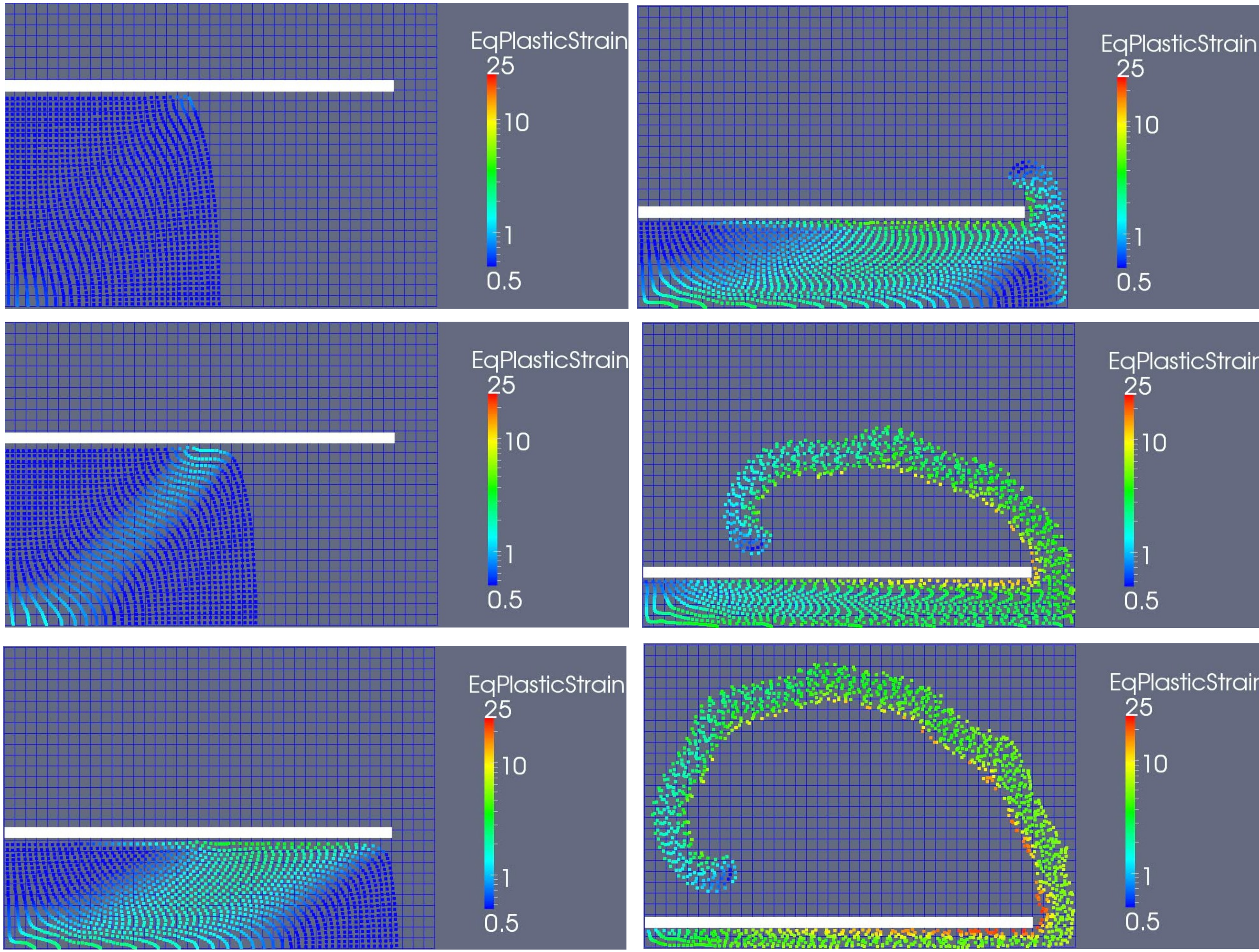
To other T-3 LANL codes

- Code development started in T-3, LANL (Los Alamos National Laboratory) since the 1960's. (KIVA, CHAD, CFDLIB, …)
- CartaBlanca is a **research** code, built on the experience learned from other code efforts, and with the advanced multiphase flow theory and numerical methods.
- Material and chemical reaction model libraries for CartaBlanca are being built as it is applied to more problems.

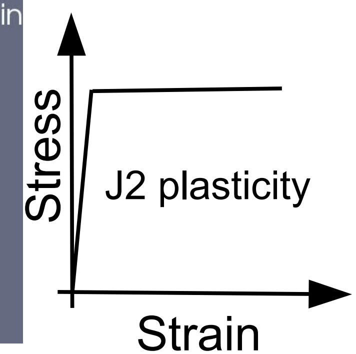
To Commercial codes

- FLUENT
  - Eulerian code. Good for flows with relatively simple constitutive relations.
- ABAQUS
  - Finite element Lagrangian code. Good for solid with small to moderate deformations.
- CartaBlanca
  - Multiphase flow, multi-material interaction code.
  - Eulerian method with Lagrangian points.
  - Fluid-structure interactions with large solid deformation.
  - Especially when material response is highly complex and nonlinear.

Plastic flow of squeezed ductile material



Similar to Bingham fluid.



When not to use CartaBlanca

1. Single or disperse multiphase flows with simple models: e.g. newtonian fluid (FLUENT).
2. Solid mechanical problems with small to moderate deformation (ABAQUS).
3. Need baroque graphic input and output.

When to use CartaBlanca

1. Need source code to implement new models.
2. Complex multi-physics problems. (Multiphase flows, coupled chemical reactions, energy and species transport, fluid-structure interactions, non-traditional fluids).
3. Solid mechanical problems with very large deformation.
4. Need to accurately track material interfaces and history variables.

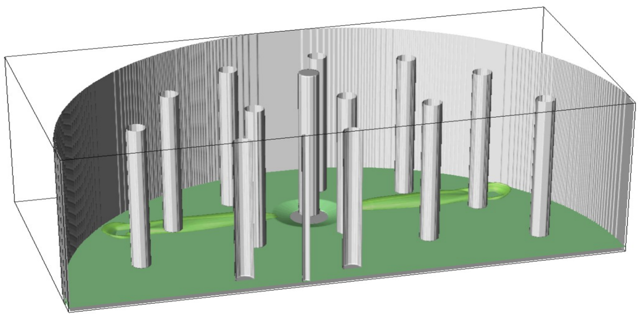
How CartaBlanca Can Help model Non-newtonian tanks

Most models for multiphase flows are restricted to disperse multiphase flows.

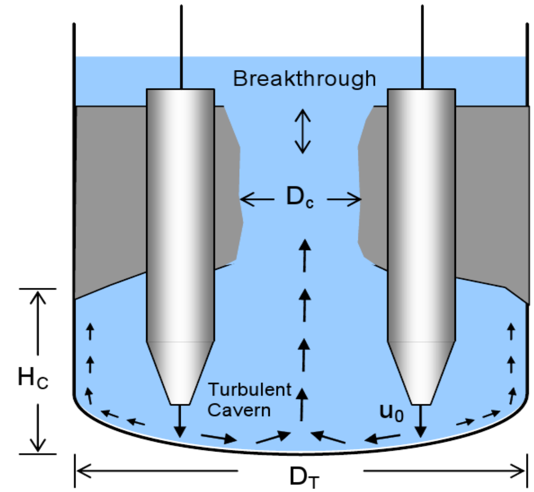
FSVT problems seem to involve a transition from a “solid” phase to a disperse phase.

Once it becomes a disperse two-phase flow, many codes, such as FLUENT, should be able to calculate it well.

Modeling of the transition from a solid phase to a disperse phase is the key.



DR Rector, (2013) PNNL



Mayer, et al. (2005) PNNL report, PNWD-3677 WTP-RPT-127